String Picture of a Frustrated Quantum Magnet and Dimer Model

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We map a geometrically frustrated Ising system with transversal field generated quantum dynamics to a strongly anisotropic lattice of non-crossing elastic strings. The combined effect of frustration, quantum and thermal spin fluctuations is explained in terms of a competition between intrinsic lattice pinning of strings and topological defects in the lattice. From this picture we obtain analytic results for correlations and the phase diagram which agree nicely with recent simulations.

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The interplay of quantum and thermal fluctuations in geometrically frustrated magnets raise new and fascinating issues both from a theoretical and experimental perspective [1, 2]. Frustration prohibits the formation of a collinear Néel state, inducing a macroscopic degeneracy of the classical ground-state. Even for magnets with a discrete Ising symmetry, the complexity of the ground-state manifold may endow the system with a continuous symmetry. Such symmetry is of particular importance to 2D quantum magnets at low temperatures since then the Mermin-Wagner theorem applies, precluding an ordered phase [3]. Another possible but contrary scenario is "order-from-disorder" where zero-point fluctuations select a small particularly susceptible class of the ground-state manifold and yield an ordered symmetry-broken state [4]. This poses the question if competing fluctuations about the classical ground-states can lead to new strongly correlated states and (quantum) phase transitions of unexpected universality classes.

The possibly simplest realization of classical frustration is provided by the antiferromagnetic Ising model on a triangular lattice (TIAF). This model is disordered even at zero temperature with a finite entropy density and algebraic decaying spin correlations [5]. Quantum dynamics arise if a magnetic field is applied transverse to the spin coupling. For this transverse field TIAF, and its companions on other 2D lattices, Moessner and Sondhi have argued the existence of both ordered and spin liquid phases [4, 6]. Experimental realizations of these models can be found either directly in magnets with strong anisotropy, e.g., in $LiHoF_4$ [7], or indirectly (via a related (2+1)D classical model) in stacked triangular lattice antiferromagnets [8] with strong couplings along the stack as studied in recent experiments on $CsCoBr_3$ [9]. Transverse field Ising models also describe the singlet sector below the spin gap of frustrated antiferromagnetic quantum Heisenberg models [10] and phases of quantum dimer models (QDM) on the dual lattice whose ordering depends on the lattice structure [11]. Interestingly, a disordered QDM appears to be a promising candidate for quantum computing [12].

In this Letter we explain the effect of simple quantum dynamics on a frustrated Ising model by mapping the transversal field TIAF to a stack of 2D lattices of non-crossing elastic strings. We show that the strings are described by a frustrated 3D XY model with a 6-fold clock term. Since our mapping yields the XY coupling constants, we can compute explicitly the phase diagram at *arbitrary* transverse field strength. The diagram is shown in Fig. 2. Previous studies of the model started from a Landau-Ginzburg-Wilson (LGW) theory [13], which neglects frustration [14], to describe the vicinity of the quantum critical point at strong transverse fields [4]. If the phase of the complex LGW order parameter is identified with the string displacement, the LGW and string actions agree except for frustration. However, the string approach shows that the configuration space is restricted since strings cannot cross each other which constrains their displacement. Moreover, the LGW approach does not provide the coupling constants, including the sign of the clock-term which is important for the selection of the ordered state. Very recent Monte Carlo simulations support the LGW prediction for the phase diagram but the computations were performed for the related (2+1)D classical model whose equivalence to the quantum problem involves a singular scaling limit which makes simulations difficult [6]. Recently, the weak field behavior has been studied in terms of a quantum kink crystal [15].

Model for magnet, dimers, and strings.—The transverse field TIAF has the Hamiltonian

$$H = J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z + \Gamma \sum_i \sigma_i^x \,, \qquad (1)$$

with nearest neighbor coupling J, transverse field Γ, and Pauli operators σ^x, σ^z. First, we will consider the classical ground states for $\Gamma = 0$ which have one frustrated bond per triangle. A complete dimer covering of the dual hexagonal lattice is obtained if a dimer is placed across each frustrated bond [16], see Fig. 1(a). For each dimer configuration a height profile h can be defined on the triangular lattice sites as follows. Starting at an arbitrary site with some integer number, one follows a triangle pointing down clockwise and changes the height by +2 (-1) if a (no) dimer is crossed. Repeating this process for all down pointing triangles, one obtains a consistent height on all sites, see Fig. 1(d). The string representa-

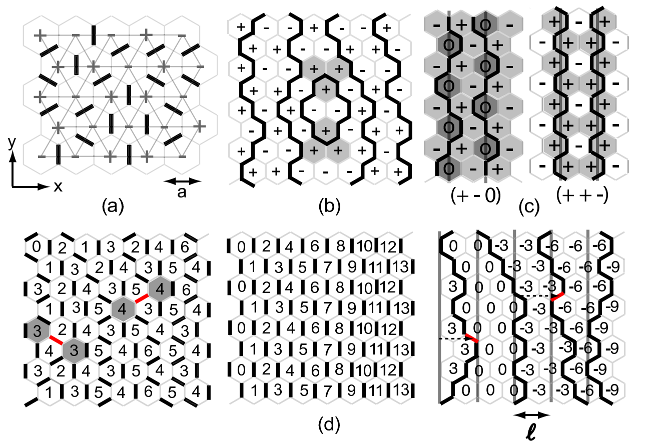

FIG. 1: (color online) (a) Relation between spins and dimers (b) Vortex–anti-vortex pair. (c) The two flat states with flippable plaquettes (grey). (d) Mapping of dimers to strings where the numbers denote the height profiles. The string displacement (arrows) is determined by the height of the two plaquettes (grey) which are joined by the displaced dimer.

tion follows from a given dimer state by the subtraction of a fixed reference state with all vertical bonds occupied [17], see Fig. 1(d). The strings fluctuate but remain directed (along the reference direction) and non-crossing (due to the frustration of the spin system). They act as domain walls across which the height (after subtraction of the reference height) changes by 3. A shift of h by 3 corresponds to a string translation by a mean string separation $\ell = 3a/2$ with a the triangular lattice constant. Thus the string displacement is $u = \ell h/3 + u_0$ with h the coincident (original) height of two hexagonal plaquettes which are joined by the displaced (non-vertical) string segment, cf. Fig. 1(d). u_0 is a global constant which differentiates between two non-equivalent states of flat strings that are not related by shifts by a lattice vector of the triangular lattice, see Fig. 1(c). For $u_0 = n\,a/2$, $n \in \mathbb{Z}$, the spins have orientations $(+\,+\,-)$ on the three sublattices and the non-vertical dimers sit on straight lines that are locked *between* the triangular lattice sites. $u_0 = a/4 + n\,a/2$ selects orientations $(+\,-\,0)$ with the straight lines locked *on* the sites, i.e., one sublattice has alternating spins as indicated in Fig. 1(c) by plaquettes with a zero.

By coarse-graining one obtains a continuous field $u(\mathbf{r})$ which allows to write the effective *free* energy of long-wavelength fluctuations of the string lattice in the form of a continuum elastic energy,

$$\mathcal{F}_{\rm el} = \int d^2\mathbf{r} \left\{ \frac{c_{11}}{2}(\partial_x u)^2 + \frac{c_{44}}{2}(\partial_y u)^2 + V_L(u) \right\} \qquad (2)$$

with compression (c_{11}) and tilt (c_{44}) modulus which are both of entropic origin. $V_L(u)$ is a periodic potential which reflects the discreteness of the lattice. Since equivalent flat states are related by shifts of all straight lines by $a/2$ and $u = ah/2 + u_0$, the locking potential must favor integer h,

$$V_L = -v\cos(2\pi h) = -v\cos\left(4\pi(u-u_0)/a\right) \qquad (3)$$

with $v > 0$ [18]. For $\sqrt{c_{11}c_{44}} > 2\pi/a^2$ the potential V_L is relevant (under renormalization) and the strings lock into that state which maximizes the entropy by allowing for local fluctuations that do not push the strings out of a tube of width ℓ around their straight reference position, i.e., $|u| \le \ell/2$. This condition restricts spin flips to certain plaquettes [grey in Fig. 1(c)]. Taking into account that strings are directed and non-intersecting, we find for a lattice of N sites that the states of orientation $(+\!-\!0)$ and $(+\!+\!-)$ allow for $2^{N/3+N/12} = \exp(0.2888\,N)$ and $18^{N/12} \times 2^{(13/18)^3 N/6} = \exp(0.2844\,N)$ localized configurations, respectively. Thus $(+\,-\,0)$ is selected and $u_0 = -a/4$ in Eq.(3).

The classical spin correlations can be easily obtained within the string picture. They follow from the local string density $\rho(\mathbf{r}) = \rho\,(1 - \partial_x u(\mathbf{r}))$ with $\rho = 1/\ell$ as $\langle\sigma_i\sigma_j\rangle = \langle e^{i\pi\int_{x_j}^{x_i}\rho(\mathbf{r})dx}\rangle$. The compression modulus in Eq. (2) can be obtained from the equivalence of non-crossing strings to 1D free Fermions [19] which is based on the Pauli principle and yields $c_{11} = \pi^2\rho^3/g$ with $g = \rho c_{44}$ the string tension. Then the periodic potential V_L is irrelevant since $\sqrt{c_{11}c_{44}} = \pi\rho^2 < 2\pi/a^2$. g can be obtained from a random walk argument, however, its actual value is unimportant since the mean squared displacement $\langle[u(\mathbf{r}) - u(\mathbf{0})]^2\rangle = 1/(\pi\sqrt{c_{11}c_{44}})\ln r$ becomes independent of g. This yields the known exact result [20]

$$\langle\sigma_i\sigma_j\rangle = \left(\frac{r_{ij}}{a}\right)^{-\eta}\cos\frac{2\pi r_{ij}}{3a}, \quad \eta = \frac{1}{2}\,. \qquad (4)$$

String model.— Now we consider a finite transversal field. First, we use the Suzuki–Trotter theorem to express the partition function of Eq. (1) in terms of a $(2+1)$D *classical* Ising model with reduced Hamiltonian [21]

$$H_{3D} = \sum_{<ij>,k=1}^{n} \tilde{K}_\parallel \sigma_{ik}\sigma_{jk} - \sum_{i,k=1}^{n} \tilde{K}_\perp \sigma_{ik}\sigma_{ik+1} \qquad (5)$$

which consists of n antiferromagnetic triangular lattices with $\tilde{K}_\parallel = J/(nT)$ which are coupled ferromagnetically with $\tilde{K}_\perp = \frac{1}{2}\ln(nT/\Gamma)$. The correspondence becomes exact for an infinite Trotter number $n \to \infty$. Next, we relate the classical spins $\sigma_{ik} = \pm 1$ to the height profile h_{ik} which is defined for each layer as above. The starting height is fixed at one site in each layer by setting $h_{0k} = 0$, (3) if $\sigma_{0k} = +1$, (-1) along a column with layer index k. Then the height on all sites is fixed (modulo 6) for a given spin state since parallel (antiparallel) spins imply a change of h by $+2$ (-1) from site to site if the down pointing triangles are traversed clockwise. If one spin is flipped, h changes on that site by ± 3. One easily proofs that these rules are met by the relation

$\sigma_{ik} = \cos(\mathbf{Q}\mathbf{R}_{ik} + \pi h_{ik}/3) = \pm 1$ with $\mathbf{Q} = (4\pi/(3a), 0, 0)$ and lattice sites $\mathbf{R}_{ik}$. The intra-layer coupling maps to $-\cos[\frac{\pi}{3}(h_{ik} - h_{jk} + \eta_{ij})]$ with a shift $\eta_{ij} = +1, -1$ for in-plane bond directions $(a, 0)$, $(a/2, \pm\sqrt{3}a/2)$, respectively. For the inter-layer coupling $\eta_{ij} = 0$. In each layer the spin states map again to a string lattice which, however, now contains vortex–anti-vortex pairs formed by triangles with 3 frustrated bonds which span string loops, see Fig. 1(b). Notice that the strings remain non-crossing since a triangle can have either 1 or 3 frustrated bonds. Including the lock-in potential of Eq.(3) with $u_0 = -a/4$ and since $h = 3(u - u_0)/\ell$, we obtain the reduced 3D string Hamiltonian

$$H_S = -\tilde{K}_\parallel \sum_{<ij>,k} \cos\left[\frac{\pi}{\ell}(u_{ik} - u_{jk} + \eta_{ij} a/2)\right] - \tilde{K}_\perp \sum_{i,k} \cos\left[\frac{\pi}{\ell}(u_{ik} - u_{ik+1})\right] + v \sum_{i,k} \cos\left[\frac{6\pi}{\ell} u_{ik}\right] \quad (6)$$

with $v > 0$ and the shift η_{ij} reflecting frustration. Since u_{ik} can vary over the bonds of a triangle only by $+a$ or $-a/2$, the energy is minimized for a non-uniform change of u_{ik} along the triangles which is distinct from a continuous field whose oriented uniform change defines a helicity, giving rise to a $\mathbb{Z}_2$ symmetry [22]. Thus the Ising model of Eq.(5) maps to a stack of 2D lattices of *non-crossing* strings which is described by a (2+1)D frustrated XY model with a 6-fold clock term. This resembles the GLW theory [13] if the string displacement is identified with the phase ϕ of the order parameter via $\phi = \pi u/\ell$. However, there are two important differences. (i) the in-plane XY coupling is frustrated and (ii) there is a topological constraint on ϕ since u is restricted by the non-crossing condition which increases the phase stiffness on large length scales. The XY coupling allows for vortex loops which are in general superpositions of two types. Vortex-anti-vortex pairs [cf. Fig. 1(b)] occurring in many layers form loops oriented perpendicular to the planes, while the boundaries of 2D regions along which strings in adjacent planes are shifted by 2ℓ form parallel loops. If the loop size is bound, the XY couplings of Eq. (6) can be expanded in u_{ik}, and each layer is described by Eq. (2) with a harmonic interlayer coupling which can render the lock-in potential relevant.

Phase diagram.— First, we note that the layers cannot decouple independently from the vortex unbinding transition in the layers since parallel loops of diverging size can occur only at a critical value for the effective $K_\parallel$ which is by factor of 1/8 below that for the in-plane dissociation of vortices [23]. In addition, a p-fold clock term is irrelevant under renormalization if $p \gtrsim 3.4$ [24], and thus we expect a quantum phase transition in the 3D XY universality class. To locate the transition, we factorize the partition function of Eq. (6) into a spin wave and a vortex part by the substitution $\tilde{K}[\cos(\phi) - 1] \to \sum_{m=-\infty}^{\infty} \exp[-K(\phi - 2\pi m)^2/2]$, denoted as Villain coupling [25]. The couplings K are known in two limits, $K = \tilde{K}$ for $\tilde{K} \to \infty$ and $K = 1/(2\ln(2/\tilde{K}))$ for $\tilde{K} \to 0$. In fact, these limits are realized for $\tilde{K}_\perp$ and $\tilde{K}_\parallel$ at large Trotter numbers n, leading to

$$K_\perp = \frac{1}{2}\ln(nT/\Gamma), \quad K_\parallel = \frac{1}{2}\ln^{-1}(2nT/J). \quad (7)$$

At $T = 0$, one can set $T \sim J/n$ so that for $n \to \infty$ the coupling $K_\perp$ remains finite, and the system shows 3D behavior. For any finite T, however, $K_\perp$ must diverge with n and the system behaves effectively as 2D on large length scales. Eliminating n from Eq. (7), we obtain a relation between $K_\parallel$ and $K_\perp$ which makes the parameter space 1D. At large n, we can expand this relation, giving

$$\sqrt{K_\parallel K_\perp} = \frac{1}{2}\left[1 - \ln(2\Gamma/J)\, K_\parallel\right]. \quad (8)$$

For layered XY models, dimensional crossover scaling [26] can be used to obtain a relation between the 3D critical value K_∞^c for the in-plane coupling and the corresponding K_n^c for a system of n layers,

$$\frac{1}{n}\frac{K_\infty^c}{K_n^c} = \gamma\left(\frac{K_\parallel}{K_\perp}\right)^{1/2}\left(1 - \frac{K_\infty^c}{K_n^c}\right)^\nu \quad (9)$$

with the 3D XY exponent $\nu \approx 2/3$ and a constant γ. This yields for $n = 1$ in the limit $K_\infty^c \ll K_1^c$ the following relation between K_∞^c and K_1^c,

$$K_\infty^c = K_1^c\left(\nu + \gamma^{-1}\sqrt{K_\perp/K_\parallel}\right)^{-1}. \quad (10)$$

At the quantum critical point the classical string system of Eq.(6) is 3D and thus at $K_\parallel = K_\infty^c$ the relations of Eqs. (8) and (10) must be identical for consistency. This implies $\gamma = 1/(2K_1^c)$ and $\Gamma_c/J = \frac{1}{2}e^{\nu/K_1^c}$. The usual Kosterlitz-Thouless (KT) argument yields for the vortex unbinding transition $K_1^c = 2/\pi \times 2/\sqrt{3}$ on the triangular lattice [22], leading to $\Gamma_c/J = 1.24$. However, this estimate neglects renormalization effects due to the clock term, frustration and the non-crossing of strings which should provide a net increase of Γ_c. Interestingly, recent Monte Carlo studies suggest $\Gamma_c/J \approx 1.65$ [6]. For $\Gamma < \Gamma_c$ the clock term is relevant, and the system is ordered.

At finite temperature, 2D XY physics dominate at large scales, and KT singularities are expected [25]. Using K_∞^c from Eq. (10) in Eq.(9) with $K_\parallel = K_n^c$ we obtain the critical coupling $K_n^c(K_\perp)$ as function of $K_\perp$ and large but finite n. This result can be used to determine the vortex unbinding transition at finite T. We set $\zeta_0 \equiv e^{2K_\perp}$ so that $n = \zeta_0\Gamma/T$ in $K_n^c(K_\perp)$. The renormalization of the coupling constants $K_\perp$, $K_\parallel$ must be dependent, and from Eq. (7) the effective $K_\parallel^{\text{eff}} = 1/(2\ln(2\zeta\Gamma/J))$ where $\zeta \equiv e^{2K_\perp^{\text{eff}}}$ is the renormalized ζ_0. Now we can use $K_n^c = K_\parallel^{\text{eff}}$ and $K_\perp = K_\perp^{\text{eff}}$ and expand $K_n^c(K_\perp)$ for large

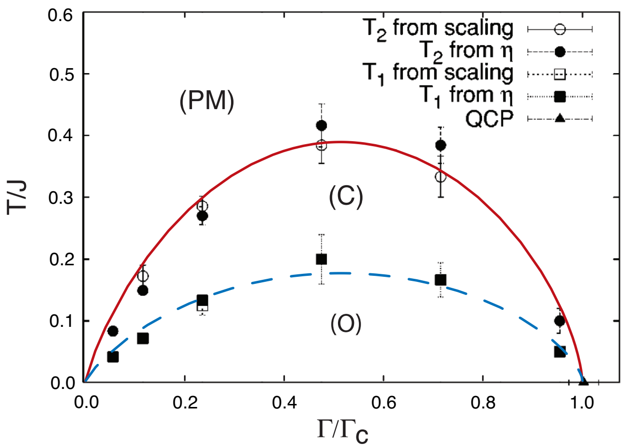

FIG. 2: (color online) Phase diagram predicted by Eq. (11) and Monte Carlo results of Fig. 1 in Ref. [6]. A critical phase (C) is separated by a boundary at $T_{c,1}$ from the paramagnetic phase (PM) and at $T_{c,2} = 4/9\, T_{c,1}$ from an ordered phase (O).

ζ which yields in the limit $n \to \infty$ the phase boundary of a critical phase (C) with bound defects,

$$\frac{T_{c,1}}{J} = b\,\frac{\Gamma}{\Gamma_c}\,\ln^{\nu}\left(\frac{\Gamma_c}{\Gamma}\right)\,, \tag{11}$$

where $b = \gamma e^{\nu/K_1^c}\zeta_0(2\ln\zeta)^{-5/3}$ is a numerical constant which is fixed by the (unknown) renormalization of $K_\perp$ and remains finite for $n \to \infty$. However, for consistency, since $\zeta_0 = nT/\Gamma$ the effective coupling must behave at large n like $K_\perp^{\rm eff} \sim (n/n_c)^{3/5}$ with a characteristic $n_c = bK_1^c(J/T)(\Gamma/\Gamma_c)$ which is a measure for the strength of quantum fluctuations and characterizes the effective system size along the Trotter ("imaginary time") axis. At a lower $T_{c,2}$ there is a second transition to an ordered state where the clock-term in Eq. (6) becomes relevant and locks the strings to the lattice. For a single layer, this transition is again of KT type with critical $\hat{K}_1^c = 9/(2\pi) \times 2/\sqrt{3}$ [25], and the boundary of the ordered phase can be obtained analogously to $T_{c,1}$ but with γ replaced by $\gamma K_1^c/\hat{K}_1^c$ in b below Eq. (11), yielding $T_{c,2} = (4/9)T_{c,1}$. Close to the quantum critical point both temperatures vanish $\sim (\Gamma_c - \Gamma)^{\nu}$ as expected from scaling. Fig. 2 compares the result of Eq. (11) to recent Monte Carlo data for the phase boundaries, showing very good agreement across the entire range of Γ for $b = 0.98$. The spin correlations in phase C decay according to Eq. (4) with η varying continuously between $\eta = 1/4$ at $T_{c,1}$ and $\eta = 1/9$ at $T_{c,2}$ [25]. At the quantum critical point one has the 3D XY result $\eta \approx 0.040$ [27]. The ordered phase (O) is characterized by finite sublattice magnetizations $(\sqrt{3}/2, -\sqrt{3}/2, 0)$ which follows from $\sigma_{jk} = \cos(\mathbf{QR}_{jk} + 2\pi(u_{jk} - u_0)/3) = \cos(\mathbf{QR}_{jk} + \pi/6)$ for flat strings ($u_{jk} = 0$) with $u_0 = -a/4$ in class $(+-0)$. This kind of order is consistent with simulations [6].

An exciting perspective is that the string analogy applies also to frustrated Ising systems with general couplings and quenched disorder examined in recent experiments [28]. A glassy state of the strings, similar to a vortex glass [29], would be an interesting possibility.

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